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* * * * * Welcome to STN International * * * * *

NEWS 1 Web Page for STN Seminar Schedule - N. America
NEWS 2 MAY 01 New CAS web site launched
NEWS 3 MAY 08 CA/CAPLUS Indian patent publication number format defined
NEWS 4 MAY 14 RDISCLOSURE on STN Easy enhanced with new search and display fields
NEWS 5 MAY 21 BIOSIS reloaded and enhanced with archival data
NEWS 6 MAY 21 TOXCENTER enhanced with BIOSIS reload
NEWS 7 MAY 21 CA/CAPLUS enhanced with additional kind codes for German patents
NEWS 8 MAY 22 CA/CAPLUS enhanced with IPC reclassification in Japanese patents
NEWS 9 JUN 27 CA/CAPLUS enhanced with pre-1967 CAS Registry Numbers
NEWS 10 JUN 29 STN Viewer now available
NEWS 11 JUN 29 STN Express, Version 8.2, now available
NEWS 12 JUL 02 LEMBASE coverage updated
NEWS 13 JUL 02 LMEDLINE coverage updated
NEWS 14 JUL 02 SCISEARCH enhanced with complete author names
NEWS 15 JUL 02 CHEMCATS accession numbers revised
NEWS 16 JUL 02 CA/CAPLUS enhanced with utility model patents from China
NEWS 17 JUL 16 CAPLUS enhanced with French and German abstracts
NEWS 18 JUL 18 CA/CAPLUS patent coverage enhanced
NEWS 19 JUL 26 USPATFULL/USPAT2 enhanced with IPC reclassification
NEWS 20 JUL 30 USGENE now available on STN
NEWS 21 AUG 06 CAS REGISTRY enhanced with new experimental property tags
NEWS 22 AUG 06 BEILSTEIN updated with new compounds
NEWS 23 AUG 06 FSTA enhanced with new thesaurus edition
NEWS 24 AUG 13 CA/CAPLUS enhanced with additional kind codes for granted patents

NEWS EXPRESS 29 JUNE 2007: CURRENT WINDOWS VERSION IS V8.2,
CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 05 JULY 2007.

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 07:11:46 ON 15 AUG 2007

=> file casreact

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'CASREACT' ENTERED AT 07:11:57 ON 15 AUG 2007

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FILE CONTENT:1840 - 11 Aug 2007 VOL 147 ISS 8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

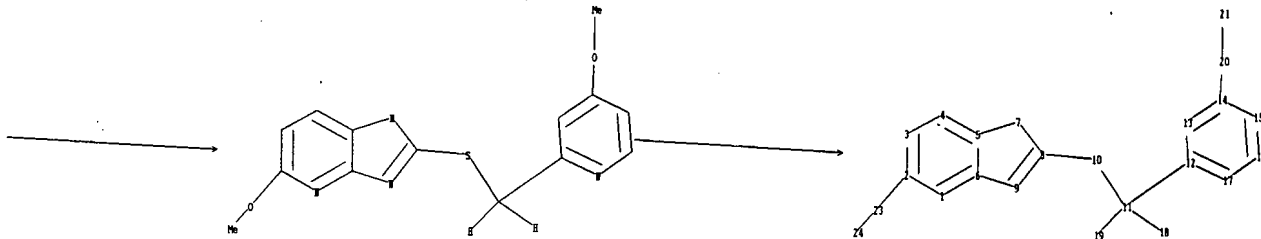
*
* CASREACT now has more than 12 million reactions *
*

Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=>

Uploading C:\Program Files\Stnexp\Queries\10561844c.str



chain nodes :

10 11 18 19 20 21 23 24

ring nodes :

1 2 3 4 5 6 7 8 9 12 13 14 15 16 17

chain bonds :

2-23 8-10 10-11 11-12 11-18 11-19 14-20 20-21 23-24

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 12-13 12-17 13-14 14-15 15-16 16-17

exact/norm bonds :

2-23 5-7 6-9 7-8 8-9 8-10 10-11 14-20

exact bonds :

11-12 11-18 11-19 20-21 23-24

normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 12-13 12-17 13-14 14-15 15-16 16-17
isolated ring systems :
containing 1 : 12 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:CLASS
20:CLASS 21:CLASS 23:CLASS 24:CLASS
fragments assigned product role:
containing 1

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 07:12:17 FILE 'CASREACT'

SCREENING COMPLETE - 0 REACTIONS TO VERIFY FROM 0 DOCUMENTS

100.0% DONE 0 VERIFIED 0 HIT RXNS 0 DOCS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED VERIFICATIONS: 0 TO 0

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1 (0 REACTIONS)

=> s l1 full

FULL SEARCH INITIATED 07:12:22 FILE 'CASREACT'

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100.0% DONE 375 VERIFIED 119 HIT RXNS 9 DOCS

SEARCH TIME: 00.00.01

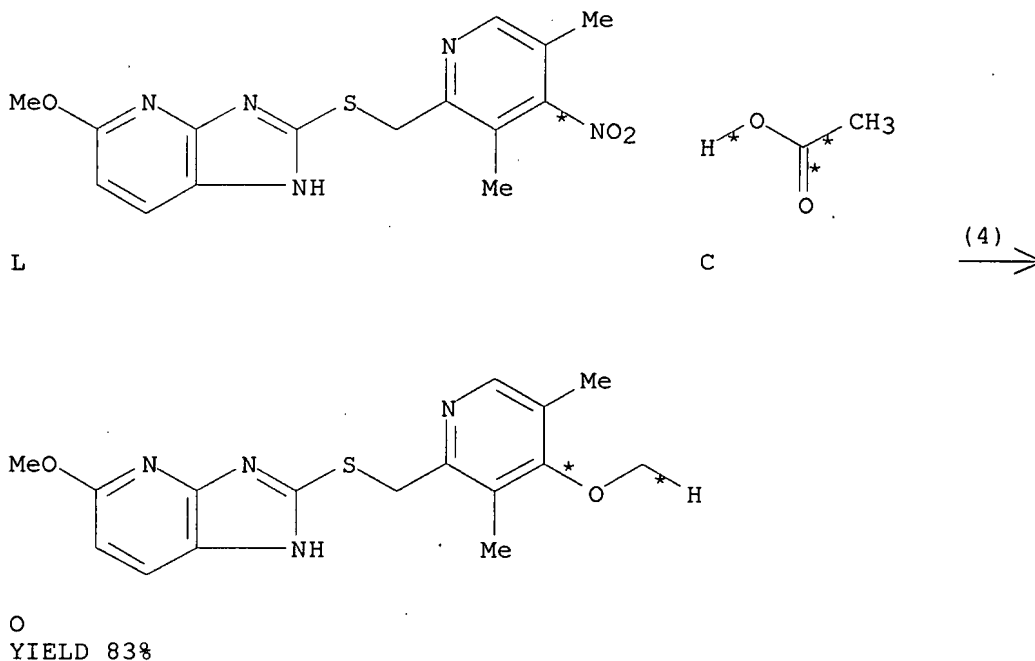
L3 9 SEA SSS FUL L1 (119 REACTIONS)

=> d bib abs fhlt tot

L3 ANSWER 1 OF 9 CASREACT COPYRIGHT 2007 ACS on STN
AN 146:45510 CASREACT
TI Synthesis of tenatoprazole
IN Dai, Liyan; Wang, Xiaozhong; Chen, Yingqi
PA Zhejiang University, Peop. Rep. China
SO Faming Zhuanli Shenqing Gongkai Shuomingshu, 10pp.
CODEN: CNXXEV
DT Patent
LA Chinese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	CN 1861600	A	20061115	CN 2006-10051971	20060614
PRAI	CN 2006-10051971		20060614		
AB	<p>The title method comprises the steps of: (1) using 2,3,5-trimethyl-4-nitropyridine N-oxide as the raw material, rearranging in the presence of anhydride at 60-120°C and hydrolyzing at 50-70°C to obtain 2-hydroxymethyl-3,5-dimethyl-4-nitropyridine, (2) reacting with chlorinating agent to obtain 2-chloromethyl-3,5-dimethyl-4-nitropyridine, (3) condensing with 2-mercapto-5-methoxyimidazo[4,5-b]pyridine at 40-65°C to obtain 2-(3,5-dimethyl-4-nitropyridine-2-methylthio)-5-methoxyimidazo[4,5-b]pyridine, (4) reacting with sodium methoxide to obtain 2-(3-5-demethyl-4-methoxypyridine-2-methylthio)-5-methoxyimidazo[4,5-b]pyridine, and (5) dissolving 2-(3-5-demethyl-4-methoxypyridine-2-methylthio)-5-methoxyimidazo[4,5-b]pyridine in halohydrocarbon and oxidating at (-25)-(-5)°C with organic peracid as the oxidant to obtain tenatoprazole.</p>				

RX(4) OF 23 ...L + C ==> O...



RX(4) RCT L 153476-67-6, C 64-19-7

STAGE(1)

SOL 67-56-1 MeOH

CON SUBSTAGE(1) 2 hours, 65 deg C

SUBSTAGE(2) 3 hours, 65 deg C

STAGE(2)

RGT C 64-19-7 AcOH

CON pH 8

PRO O 113713-24-9

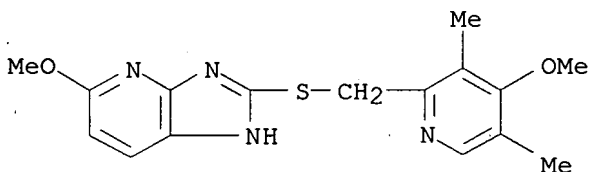
L3 ANSWER 2 OF 9 CASREACT COPYRIGHT 2007 ACS on STN
AN 144:412513 CASREACT

TI Process for the preparation of tenatoprazole salts
 IN Joshi, Ramesh Anna; Joshi, Rohini Ramesh; Wakchaure, Vijay Naryan; Gurjar, Mukund Keshav
 PA India
 SO U.S. Pat. Appl. Publ., 5 pp.
 CODEN: USXXCO
 DT Patent
 LA English
 FAN.CNT 1

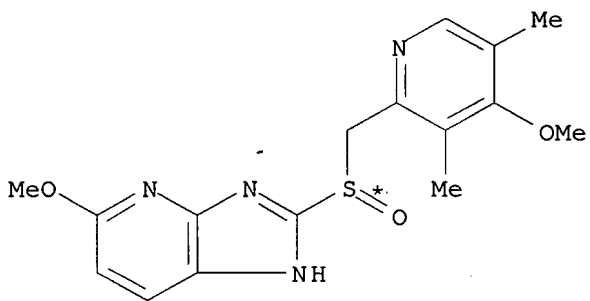
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PI	US 2006089376	A1	20060427	US 2004-973983	20041027
	US 2006089377	A1	20060427	US 2005-175027	20050706
	US 2006270711	A1	20061130	US 2006-490247	20060721
PRAI	US 2004-973983		20041027		
	US 2005-175027		20050706		

AB Li, Na, Ca, K, or Mg salts of 5-methoxy-2-(4-methoxy-3,5dimethylpyridin-2-ylmethylsulfinyl)imidazo[4,5-b]pyridine (i.e., tenatoprazole) are prepared in high yield and selectivity by oxidizing the corresponding tenatoprazole sulfide with an oxidant (e.g., m-chloroperbenzoic acid) and isolating the salt (Li, Na) by treatment with an alkali (e.g., sodium hydroxide) or exchanging the sodium salt of tenatoprazole with a Mg²⁺ or Ca²⁺ cation (e.g., by treatment of the sodium salt of tenatoprazole with calcium chloride).

RX(1) OF 7 A ==> B...



A



● Na

B
 YIELD 76%

RX(1) RCT A 113713-24-9

STAGE(1)

RGT C 584-08-7 K2CO3
 SOL 7732-18-5 Water, 67-66-3 CHCl3
 CON room temperature -> 5 deg C

STAGE(2)

RGT D 937-14-4 MCPBA
 SOL 67-66-3 CHCl3
 CON SUBSTAGE(1) 85 minutes, 0 - 5 deg C
 SUBSTAGE(2) 20 minutes, 0 - 5 deg C

STAGE(3)

RGT E 1310-73-2 NaOH
 SOL 7732-18-5 Water

PRO B 335299-59-7

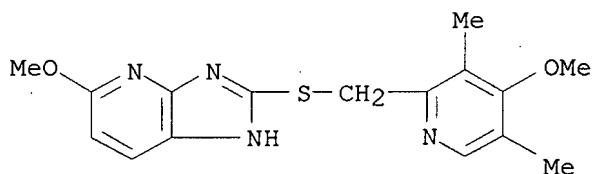
L3 ANSWER 3 OF 9 CASREACT COPYRIGHT 2007 ACS on STN
 AN 144:412510 CASREACT
 TI Process for the preparation of tenatoprazole salts
 IN Joshi, Ramesh Anna; Joshi, Rohini Ramesh; Wakchaure, Vijay Naryan; Gurjar, Mukund Keshav
 PA Council of Scientific and Industrial Research, India
 SO PCT Int. Appl., 13 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2006043280	A1	20060427	WO 2004-IN328	20041019
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
	RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			

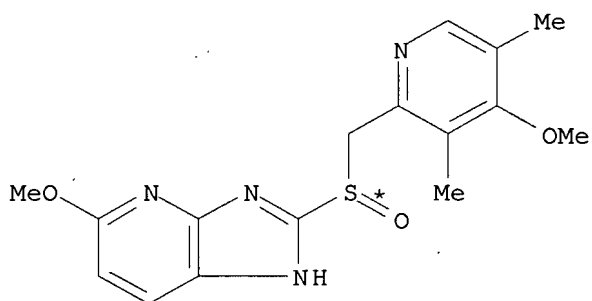
PRAI WO 2004-IN328 20041019

AB Li, Na, Ca, K, or Mg salts of 5-methoxy-2-(4-methoxy-3,5dimethylpyridin-2-ylmethylsulfinyl)imidazo[4,5-b]pyridine (i.e., tenatoprazole) are prepared in high yield and selectivity by oxidizing the corresponding tenatoprazole sulfide with an oxidant (e.g., m-chloroperbenzoic acid) and isolating the salt (Li, Na) by treatment with an alkali (e.g., sodium hydroxide) or exchanging the sodium salt of tenatoprazole with a Mg²⁺ or Ca²⁺ cation (e.g., by treatment of the sodium salt of tenatoprazole with calcium chloride).

RX(1) OF 3 A ==> B



A



● Na

B

YIELD 76%

RX(1) RCT A 113713-24-9

STAGE(1)

RGT C 298-14-6 KHCO₃, D 937-14-4 MCPBA

SOL 7732-18-5 Water, 67-66-3 CHCl₃

CON SUBSTAGE(1) room temperature -> 5 deg C

SUBSTAGE(2) 85 minutes, 0 - 5 deg C

SUBSTAGE(3) 20 minutes, 0 - 5 deg C

STAGE(2)

RGT E 1310-73-2 NaOH

SOL 7732-18-5 Water

PRO B 335299-59-7

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 4 OF 9 CASREACT COPYRIGHT 2007 ACS on STN

AN 144:370094 CASREACT

TI Process for preparation of sulfoxides, particularly tenatoprazole enantiomers and its analogs, by enantioselective oxidation using titanium(IV)-based catalyst and chiral α - or β -amino alcohol ligand

IN Cohen, Avraham; Schutze, Francois; Charbit, Suzy; Martinet, Frederic; Gizecki, Patricia

PA Sidem Pharma SA, Luxembourg

SO Fr. Demande, 22 pp.

CODEN: FRXXBL

DT Patent

LA French

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	FR 2876101	A1	20060407	FR 2004-10483	20041005
	FR 2876101	B1	20070302		
	AU 2005291156	A1	20060413	AU 2005-291156	20051005
	CA 2580446	A1	20060413	CA 2005-2580446	20051005
	WO 2006037894	A1	20060413	WO 2005-FR2447	20051005

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

EP 1802620 A1 20070704 EP 2005-804208 20051005

R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR

IN 2007DN02060 A 20070803 IN 2007-DN2060 20070316

NO 2007001524 A 20070427 NO 2007-1524 20070323

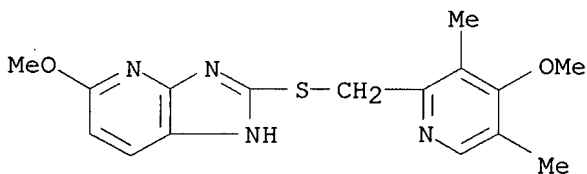
PRAI FR 2004-10483 20041005

WO 2005-FR2447 20051005

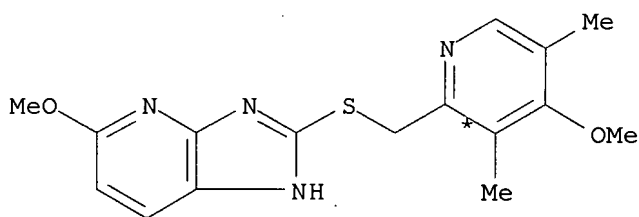
OS MARPAT 144:370094

AB The invention is related to the preparation of enantiomeric sulfoxide derivs., and their salts, particularly tenatoprazole enantiomers and its analogs, by enantioselective oxidation of sulfides of formula A-CH₂-S-B [A = substituted pyridinyl; B = (un)substituted imidazo-pyridinyl] with an oxidation agent in the presence of a Ti(IV)-based catalyst and a chiral cyclic α - or β -amino alc. ligand, followed by optional salt formation. The advantages include high enantiomeric excess (e.e.), reduced amts. of undesired sulfones, high product purity and yield. Thus, addition of Ti(IV) isopropylate, followed by cumene hydroperoxide to a solution of 5-methoxy-2-[[[4-methoxy-3,5-dimethyl-2-pyridinyl)methyl]sulfanyl]imidazo[4,5-b]pyridine and (1R,2S)-(+)-1-amino-2-indanol in anhydrous Py, and stirring the resulting mixture at 22° for 5 h gave (S)-(-)-tenatoprazole in 97% e.e. with 4% sulfone in the crude product.

RX(1) OF 2 2 A ==> B + C

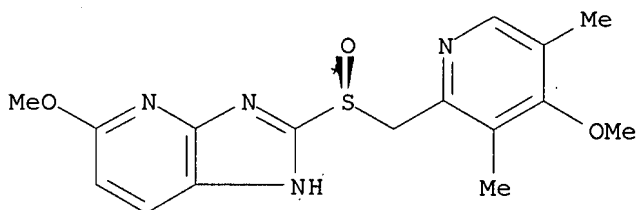


A

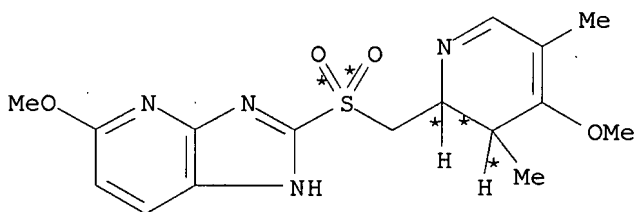


A

(1) →



B



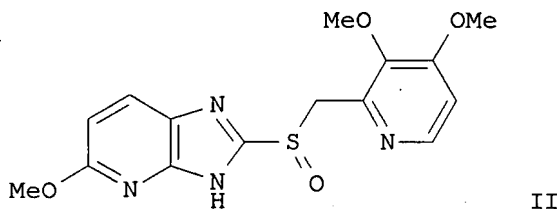
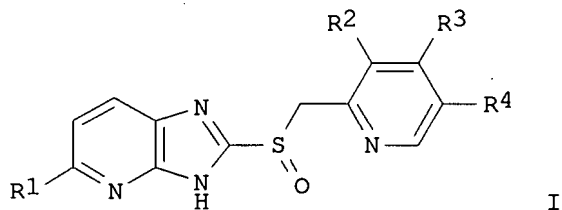
C

RX(1) RCT A 113713-24-9
 RGT D 80-15-9 Cumene hydroperoxide, E 136030-00-7 1H-Inden-2-ol,
 1-amino-2,3-dihydro-, (1R,2S)-
 PRO B 705968-86-1, C 882039-29-4
 CAT 546-68-9 Ti(OPr-i)₄
 SOL 872-50-4 NMEP
 CON 5 hours, 22 deg C
 NTE optimization study(optimized on solvent), stereoselective
 RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 5 OF 9 CASREACT COPYRIGHT 2007 ACS on STN
 AN 143:440411 CASREACT
 TI Preparation of dialkoxy imidazopyridine derivatives for treatment of
 gastrointestinal disorders
 IN Zimmermann, Peter Jan; Buhr, Wilm
 PA Altana Pharma AG, Germany
 SO PCT Int. Appl., 25 pp.
 CODEN: PIXXD2
 DT Patent
 LA English

FAN.CNT 1

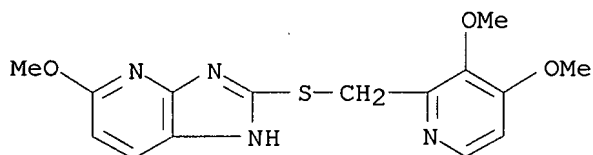
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	AU 2005238215	A1	20051110	AU 2005-238215	20050426
	CA 2563808	A1	20051110	CA 2005-2563808	20050426
	EP 1742946	A1	20070117	EP 2005-740172	20050426
	R:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, LV, MK, YU			
	CN 1946722	A	20070411	CN 2005-80012903	20050426
	NO 2006005200	A	20061113	NO 2006-5200	20061113
	IN 2006MN01407	A	20070608	IN 2006-MN1407	20061120
PRAI	EP 2004-10042		20040428		
	WO 2005-EP51851		20050426		
OS	MARPAT 143:440411				
GI					



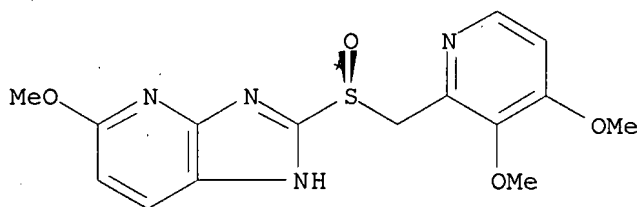
AB Title compds. I [R1 = alkoxy or cycloalkylalkoxy; R2 = alkoxy; R3 = alkoxy or alkoxyalkoxy; R4 = H or alkyl] and their pharmaceutically acceptable salts, are prepared and disclosed as treatment for gastrointestinal disorders. Thus, e.g., II was prepared by coupling of 5-methoxy-3H-imidazo[4,5-b]pyridine-2-thiol with 2-chloromethyl-3,4-dimethoxy pyridinium chloride and subsequent oxidation. The ability of I to inhibit acid secretion on the perfused rat stomach was evaluated and it was

revealed that selected compds. of the invention displayed inhibitory activity above 50%. Pharmaceutical compns. comprising I are disclosed.

RX(1) OF 3 ...2 A ==> B + C

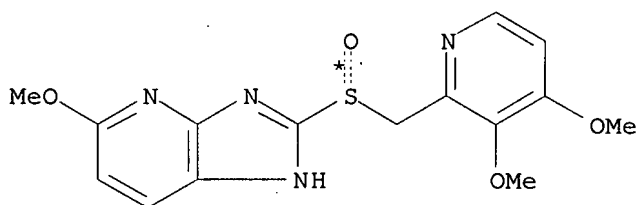


2 A



B

YIELD 63% (49)



C

YIELD 63% (51)

RX(1) RCT A 868700-13-4

STAGE(1)

RGT D 937-14-4 MCPBA

SOL 75-09-2 CH2Cl2

CON SUBSTAGE(1) -10 deg C -> 0 deg C

SUBSTAGE(2) 1 hour, 0 deg C

STAGE(2)

RGT E 7772-98-7 Na2S2O3, F 144-55-8 NaHCO3

SOL 7732-18-5 Water

CON 0 deg C

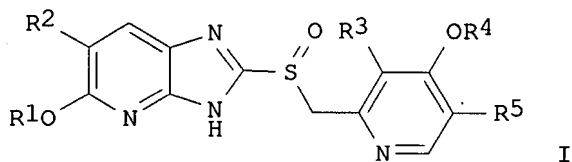
PRO B 868700-05-4, C 868700-07-6

NTE racemate resolution using chiral column chromatography on Chiralpak AS-H5

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

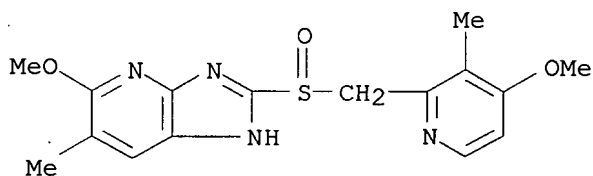
L3 ANSWER 6 OF 9 CASREACT COPYRIGHT 2007 ACS on STN
 AN 143:440408 CASREACT
 TI Preparation of imidazo[4,5-b]pyridine derivatives for treatment of
 diseases caused by gastric acid
 IN Miyazawa, Shuhei; Harada, Hitoshi; Fujisaki, Hideaki; Kubota, Atsuhiko;
 Kodama, Kotaro; Nagakawa, Junichi; Watanabe, Nobuhisa; Oketani, Kiyoshi
 PA Eisai Co., Ltd., Japan
 SO PCT Int. Appl., 120 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005103049	A1	20051103	WO 2005-JP8311	20050421
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	AU 2005235906	A1	20051103	AU 2005-235906	20050421
	CA 2562812	A1	20051103	CA 2005-2562812	20050421
	US 2005272764	A1	20051208	US 2005-110756	20050421
	EP 1737862	A1	20070103	EP 2005-737039	20050421
	R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, LV, MK, YU				
	CN 1976929	A	20070606	CN 2005-80011558	20050421
	US 2006167041	A1	20060727	US 2006-385786	20060322
	NO 2006004902	A	20061204	NO 2006-4902	20061026
PRAI	JP 2004-126533		20040422		
	US 2005-110756		20050421		
	WO 2005-JP8311		20050421		
OS	MARPAT 143:440408				
GI					



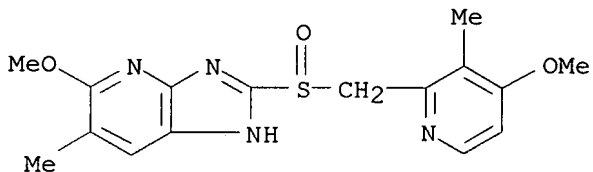
AB Title compds. represented by the formula I [wherein R1 = (un)substituted (cyclo)alkyl, alkenyl, alkynyl or phenyl; R2 = H or alkyl; R3 = Me or Et; R4 = alkyl; R5 = H; and their salts or hydrates thereof] were prepared For example, II (I: R1-R4 = Me, R5 = H) was provided in a multi-step synthesis starting from 2-fluoro-3-methylpyridine. II showed inhibition of gastric acid secretion in rat with 79% inhibition rate, and were tested for cytochrome P 450 gene induction in human cryopreserved hepatocytes. Thus, I and their pharmaceutical compns. are useful for the treatment of the disease caused by gastric acid, such as gastric ulcer.

RX(1) OF 282 ...A ==> B



A

(1) \longrightarrow



● Na

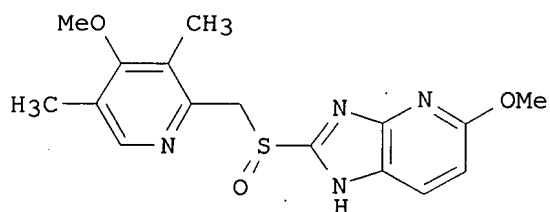
B

YIELD 99%

RX(1) RCT A 868539-24-6
RGT C 1310-73-2 NaOH
PRO B 868539-19-9
SOL 7732-18-5 Water, 64-17-5 EtOH
CON 30 minutes, room temperature
RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 7 OF 9 CASREACT COPYRIGHT 2007 ACS on STN
AN 142:430268 CASREACT
TI Preparation of (S)- and (R)-enantiomers of tenatoprazole as H⁺/K⁺ ATPase inhibitors
IN Li, Shuxin; Zhao, Yanjin; Guo, Jinhua
PA Institute of Radiomedicine, Academy of Military Medical Science of PLA, Peop. Rep. China
SO Faming Zhuanli Shenqing Gongkai Shuomingshu, 9 pp.
CODEN: CNXXEV
DT Patent
LA Chinese
FAN.CNT 1

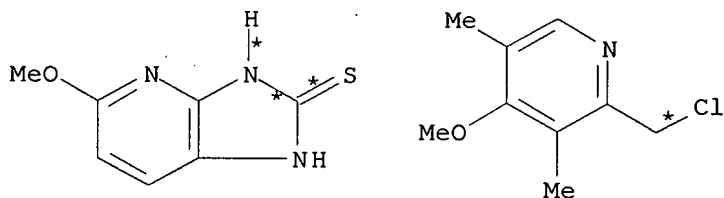
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	CN 1453278	A	20031105	CN 2002-117637	20020510
PRAI	CN 2002-117289		20020423		
GI					



I

AB The invention is related to (S)- and (R)-enantiomers of tenatoprazole I and pharmaceutically acceptable salts thereof, their preparation and uses. (S)-I was synthesized by enantioselective oxidation of the corresponding sulfide with dicumyl peroxide in the presence of (i-PrO)₄Ti and D-tartaric acid di-Et ester in 71.5% yield. (R)-I was obtained via oxidation of the corresponding sulfide with m-chloroperbenzoic acid followed by chiral HPLC resolution (37.5% yield). The two enantiomers showed stronger activity than omeprazole and comparable activity to tenatoprazole both in an inhibition assay against H⁺/K⁺ ATPase and in a gastric acid secretion-inhibition test in rat. Therefore, the invented compds. are useful for the treatment of gastric acid secretion disorders.

RX(6) OF 43 ...O + Q ==> R...

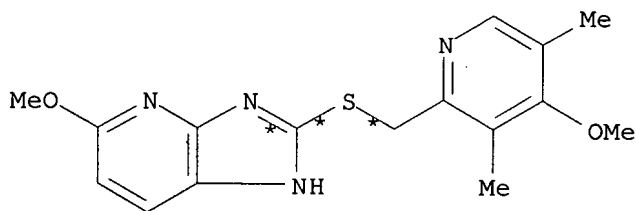


O

● HCl

Q

(6) →



R

RX(6) RCT O 113713-60-3, Q 86604-75-3

STAGE(1)

RGT S 1310-73-2 NaOH

SOL 7732-18-5 Water, 64-17-5 EtOH

CON SUBSTAGE(1) 0.5 hours, 10 deg C

SUBSTAGE(2) 2 hours, 10 deg C
SUBSTAGE(3) overnight, room temperature

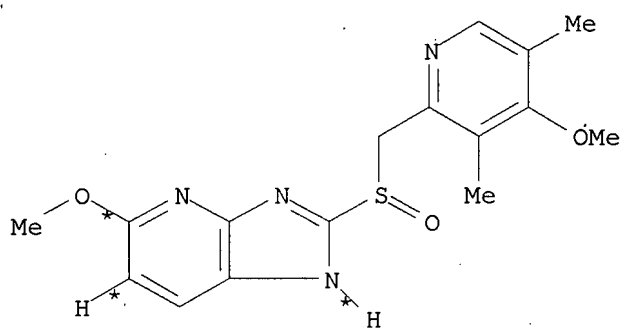
STAGE(2)

RGT P 64-19-7 AcOH
SOL 7732-18-5 Water
CON room temperature

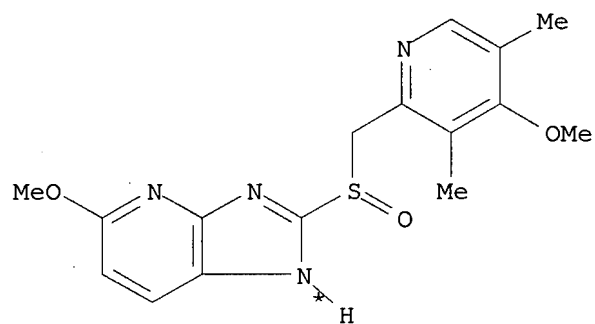
PRO R 113713-24-9

L3 ANSWER 8 OF 9 CASREACT COPYRIGHT 2007 ACS on STN
AN 141:116452 CASREACT
TI Chemistry of Covalent Inhibition of the Gastric (H⁺, K⁺)-ATPase by Proton Pump Inhibitors
AU Shin, Jai Moo; Cho, Young Moon; Sachs, George
CS Department of Physiology and Medicine, University of California, Los Angeles, CA, 90073, USA
SO Journal of the American Chemical Society (2004), 126(25), 7800-7811
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English
AB Proton pump inhibitors (PPIs), drugs that are widely used for treatment of acid related diseases, are either substituted pyridylmethylsulfinyl benzimidazole or imidazopyridine derivs. They are all prodrugs that inhibit the acid-secreting gastric (H⁺, K⁺)-ATPase by acid activation to reactive thiophiles that form disulfide bonds with one or more cysteines accessible from the exoplasmic surface of the enzyme. This unique acid-catalysis mechanism had been ascribed to the nucleophilicity of the pyridine ring. However, the data obtained here show that their conversion to the reactive cationic thiophilic sulfenic acid or sulfenamide depends mainly not on pyridine protonation but on a second protonation of the imidazole component that increases the electrophilicity of the C-2 position on the imidazole. This protonation results in reaction of the C-2 with the unprotonated fraction of the pyridine ring to form the reactive derivs. The relevant PPI pKa's were determined by UV spectroscopy of the benzimidazole or imidazopyridine sulfinylmethyl moieties at different medium pH. Synthesis of a relatively acid stable analog, N1-Me lansoprazole, allowed direct determination of both pKa values of this intact PPI
PPI allowing calcn. of the two pKa values for all the PPIs. These values predict their relative acid stability and thus the rate of reaction with cysteines of the active proton pump at the pH of the secreting parietal cell. The PPI accumulates in the secretory canaliculus of the parietal cell due to pyridine protonation then binds to the pump and is activated by the second protonation on the surface of the protein to allow disulfide formation.

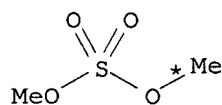
RX(15) OF 26 2 AH + 2 S ==> AI + AJ



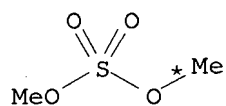
AH



AH

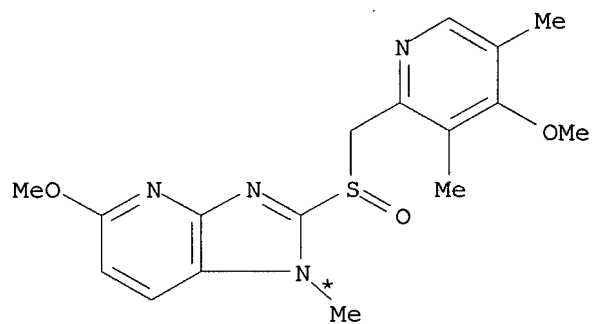


S

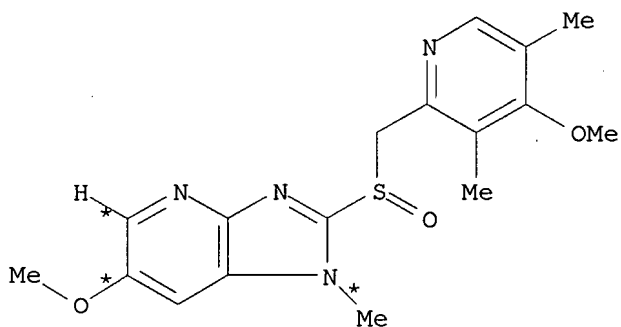


S

(15) \longrightarrow



AI



AJ

RX(15) RCT AH 113712-98-4, S 77-78-1

STAGE(1)

RGT U 6674-22-2 DBU
SOL 75-09-2 CH2Cl2
CON room temperature

STAGE(2)

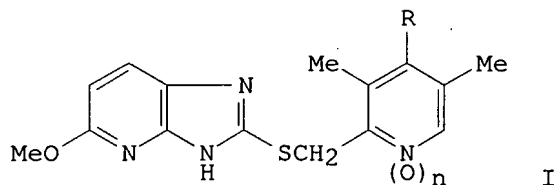
SOL 7732-18-5 Water
CON 30 minutes, room temperature

PRO AI 721924-07-8, AJ 721920-63-4

RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 9 OF 9 CASREACT COPYRIGHT 2007 ACS on STN
AN 120:164168 CASREACT
TI Preparation of 5-methoxy-2-[[[4-methoxy-3,5-dimethyl-2-pyridyl)methyl]thio]imidazo[4,5-b]pyridine and its intermediates
IN Amano, Michiaki; Takeda, Haruki
PA Tokyo Tanabe Co, Japan
SO Jpn. Kokai Tokkyo Koho, 11 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

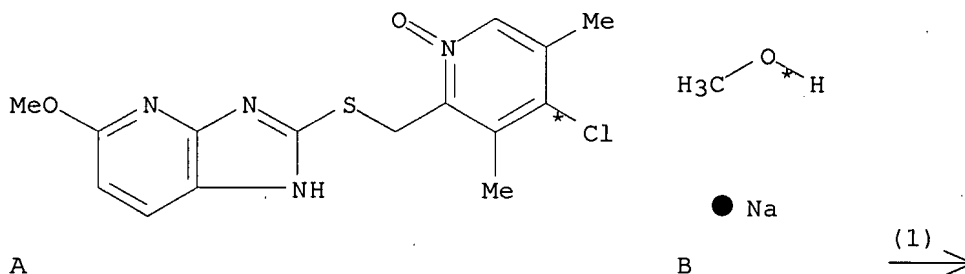
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 05222038	A	19930831	JP 1992-25002	19920212
	JP 3158599	B2	20010423		
PRAI	JP 1992-25002		19920212		
GI					



AB The title compound (I; R = MeO, n = 0) (II), useful as an intermediate for a

known antiulcer agent, 5-methoxy-2-[[4-methoxy-3,5-dimethyl-2-pyridyl)methyl]sulfinyl]imidazo[4,5-b]pyridine, is prepared Thus, 4-chloro-2-chloromethyl-3,5-dimethylpyridine N-oxide was stirred with 2-mercapto-5-methoxyimidazo[4,5-b]pyridine in EtOH at 35° for 2.5 h to give 82% I (R = Cl, n = 1) which was refluxed with NaOMe in MeOH-PhMe for 4 h to give 71% I (R = MeO, n = 1). This was stirred with PCl3 in CH2Cl2 at room temperature for 3 h to give 95% II.

RX(1) OF 15 ...A + B ==> C...



A

B

C

YIELD 71%

RX(1) RCT A 153476-63-2, B 124-41-4
 PRO C 153476-64-3
 SOL 67-56-1 MeOH, 108-88-3 PhMe
 NTE reflux

=> FIL STNGUIDE

COST IN U.S. DOLLARS

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

CA SUBSCRIBER PRICE

SINCE FILE	TOTAL
ENTRY	SESSION
159.18	159.39
SINCE FILE	TOTAL
ENTRY	SESSION
-6.57	-6.57

FILE 'STNGUIDE' ENTERED AT 07:14:15 ON 15 AUG 2007
 USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
 COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

FILE CONTAINS CURRENT INFORMATION.
 LAST RELOADED: Aug 10, 2007. (20070810/UP).

=> d his

(FILE 'HOME' ENTERED AT 07:11:46 ON 15 AUG 2007)

FILE 'CASREACT' ENTERED AT 07:11:57 ON 15 AUG 2007

L1 STRUCTURE UPLOADED
L2 0 S L1
L3 9 S L1 FULL

FILE 'STNGUIDE' ENTERED AT 07:14:15 ON 15 AUG 2007

=> log y

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
1.02	160.41

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-6.57

CA SUBSCRIBER PRICE

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